Center for Applied Scientific Computing

# Nonlinear Solvers and Differential Equations

## Algorithms and Software for Solution of Large-scale Nonlinear Problems and Sensitivities

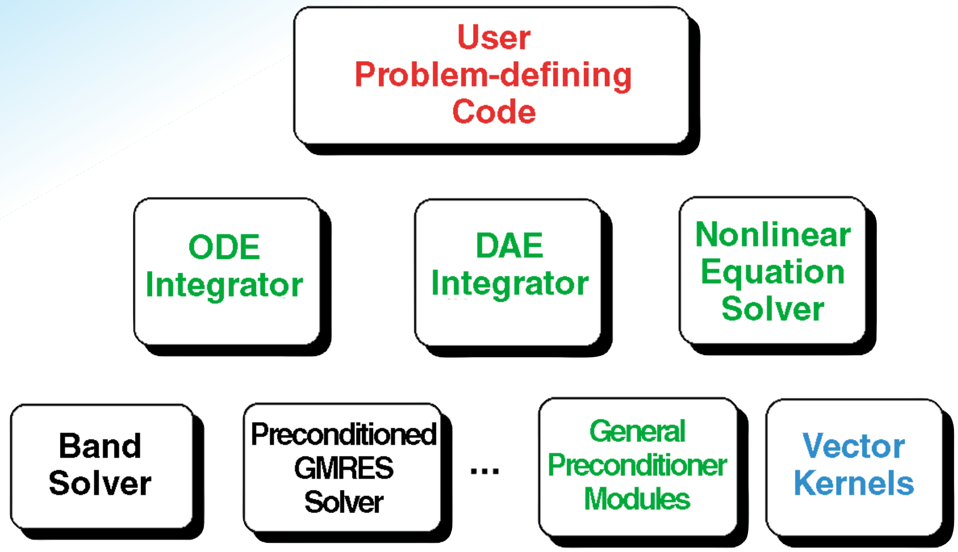


*Figure 1. The integrator PVODE, nonlinear system solver KINSOL, and the related differential–algebraic system solver IDA use a modular and extensible design.*

The Nonlinear Solvers and Differential Equations (NSDE) project at the Center for Applied Scientific Computing (CASC) focuses on research and development of solvers and sensitivity analysis techniques for nonlinear, time-dependent, and steady-state partial differential equations. We are implementing our methods into a suite of software codes: CVODE/PVODE for systems of ordinary differential equations (ODEs); IDA for differential-algebraic systems (DAEs); and KINSOL for nonlinear systems of equations. Current and future research is concentrating on the use of our time-integrators and nonlinear solvers together with sensitivity analysis techniques in the development of uncertainty quantification, model evaluation, and optimization techniques for nonlinear systems, as well as the combination of optimization under uncertainty.

### Nonlinear Methods

Powerful, massively parallel supercomputers and highly effective solvers have cleared the way to solving fully implicit formulations of many nonlinear application models. Solutions to fully implicit formulations provide more accuracy and, due to the ability to take larger time steps in resolving time-dependent behavior, can be faster than explicit formulations.

We conduct research in the solution of implicit nonlinear differential equations discretized on large, three-dimensional meshes. This work examines parallel solution strategies for nonlinear discrete systems arising from solving a steady-state problem or from solving a time step within an implicit, time-dependent problem. Investigators also pursue solution strategies for the linear systems arising in each nonlinear iteration.

Our initial focus has been in the application of Newton–Krylov methods for solving nonlinear systems. These methods can achieve quadratic convergence of the nonlinear iteration, provided the linear systems have been solved sufficiently and accurately. One difficulty, however, arises in iterating the linear solver to a low enough tolerance, a requirement that often necessitates an efficient and scalable preconditioner for the Krylov method. We have been investigating various multigrid methods applied as preconditioners for these systems.

Our methods have been used to solve a 746-million unknown fully implicit nonlinear diffusion problem on 5,832 processors of the ASCI Red machine. We have shown that the Newton–Krylov-multigrid methods have excellent scaling properties on these large problems and that the fully implicit formulation with this solver is faster and more accurate than popular semi-implicit methods.

Additionally, we are investigating nonlinear multigrid schemes such as the Full Approximation Storage (FAS) method for nonlinear elliptic and parabolic problems. These schemes provide an alternative to the Newton–Krylov approach. While FAS methods may require less storage than Newton–Krylov schemes, they are not as fully understood. We are examining these methods and comparing the resulting performance to that of the Newton–Krylov-multigrid methods.

### Sensitivity Analysis

In many applications we are interested in quantifying the influence of changes in model parameters on the simulation solution. To assess the first-order sensitivity of the simulations, we are developing forward methods and adjoint sensitivity methods.

Forward sensitivity methods can be formulated in terms of an ODE, a DAE, or an algebraic equation (for steady problems) for the solution sensitivities with respect to a fixed set of parame-



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ters. By appending these equations to the original system, the state solution and sensitivities can be solved simultaneously by the simulation code. The additional sensitivity equations contain terms involving Jacobian matrix-vector products and partial derivatives. These quantities can be evaluated either with finite differences or, as a more efficient and exact alternative, through the use of automatic differentiation (AD) techniques.

In cases where the sensitivity of the solution is needed with respect to a large number of parameters, adjoint methods may prove more efficient than forward methods. This approach involves formulating and solving adjoint equations. Again, either finite differences or AD can be used to evaluate the adjoint equations. Both approaches rely on the ability to efficiently store or recompute the simulation in the forward direction. We are researching reduced basis methods, where only a subset of the simulation results are stored and interpolation schemes are used to express the solution in terms of this subset.

We have applied forward sensitivity analysis techniques for both neutral particle transport and cloud parcel microphysics models. In the latter case, the solution sensitivities determined the relative importance of input parameters into the model. In the former case, sensitivities quantified solution uncertainties with the same accuracy, but much faster than with Monte Carlo techniques.

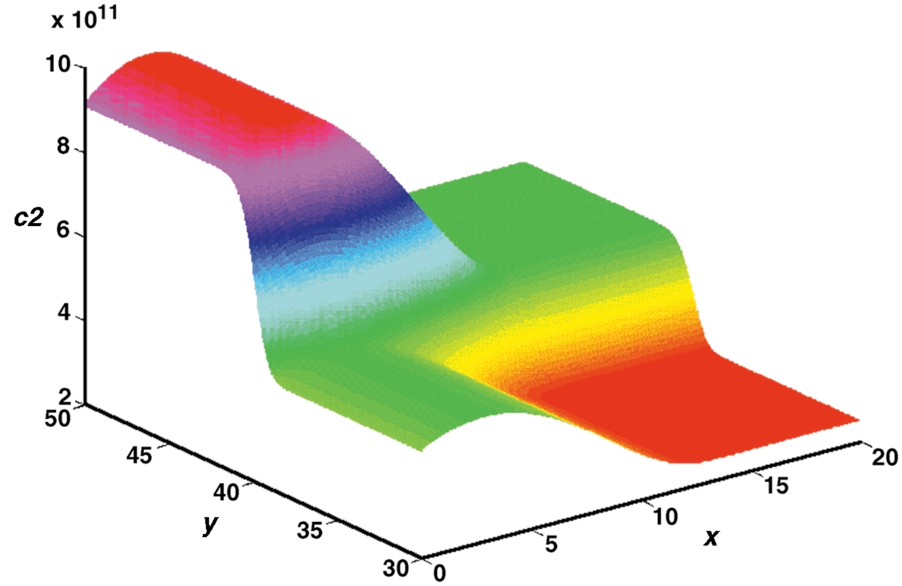


*Figure 2. One species surface solution from a 400 × 400 mesh PVODE run of a simplified ozone reaction transport model.*

## Software

General-purpose (sequential) software packages developed at Lawrence Livermore National Laboratory (LLNL) for the three problem classes of ODEs, DAEs, and nonlinear systems are among the most widely used solvers anywhere. One such package is a C-language solver called CVODE. Its highly modular structure was designed with parallel extensions in mind. A parallel solver for ordinary differential equation systems, called PVODE, builds upon CVODE by way of parallelization of the module of vector kernels, using the Single Program, Multiple Data (SPMD) programming model. PVODE contains two method options, namely, the nonstiff method and the stiff method with iterative solution of the linear systems. Likewise, our C-language nonlinear system solver, KINSOL, has been extended to a parallel version, sharing with PVODE the linear solver and vector kernels. It uses Inexact Newton methods, coupled with a line-search strategy to enhance global convergence and preconditioned iterative methods for the linear systems. Building on other widely used LLNL software, we have developed IDA, an analogous C-language parallel version of a DAE system solver, again sharing PVODE's linear solver and vector modules. Both PVODE and KINSOL include a set of interface routines for a Fortran calling program and problem-defining routines.

In all codes, the nonlinear systems are treated by a Newton iteration, which requires the solution of linear systems that are typically large and sparse. For such systems, iterative (Krylov subspace) methods are an attractive choice, but to be robust these methods require preconditioning. We are developing preconditioner modules for use with PVODE, KINSOL, and IDA based on banded and sparse Jacobian matrix approximations, including automatic generation (in parallel) of required matrix data. One such module has been completed. It uses a block-diagonal preconditioner matrix with banded blocks, built from a pair of user-supplied routines -- for an approximation to the system function and associated communication. This approach is based on domain decomposition methodology for partial differential equations. Eventually, our FAS methods will be implemented as a nonlinear solver in these codes as well.

## Applications

PVODE is being used in a parallel 3D tokamak turbulence model in the LLNL Magnetic Fusion Energy division. KINSOL is being applied within CASC to solve a nonlinear Richards'equation for pressures in porous media flows. PVODE, KINSOL, and IDA are being used on the solution of 3D Boltzmann transport problems within CASC. The sensitivity versions of all three have been used to determine solution sensitivities of neutral particle transport applications with respect to various model inputs. IDA and its sensitivity version are being used in a cloud and aerosol microphysics model at LLNL to study cloud formation processes.

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*The NSDE Website is located at http://www.llnl.gov/CASC/nsde.*

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